



## **Physical Models for NIC EOS, Opacity, Transport, Nuclear, Kinetics**

**J. Wark and G. Collins**

**P. Sterne, C. Mauche, S. Hamel, B. Heeter, R. Rygg, E. Schwegler, D. Clark, S. Haan, L. Benedict, J. Gaffney, D. Fratanduono, P. Celliers, Y. Ping, O. Landen, J. Eggert, R. Marrs, C. Bellei, P. Amendt, S. Wilks, M. Akin, J. Hammer, C. Iglesias, D. Hicks, H. Scott, J. Castor, A. Lazicki, B. Wilson, T. Luu, D. McNabb, G. Zimmerman**

**Lawrence Livermore National Laboratory • National Ignition Campaign**

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

## Several physical models are important for manipulating HED matter to ignition

Laser Energy = 1.3 MJ

X-ray Energy = 1 MJ

Energy to capsule = 120 kJ  
Set adiabat

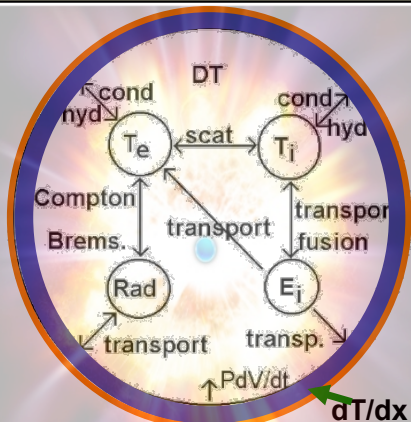
Fuel K.E. = 12 KJ, Shell K.E. ~ 20 KJ

Hot spot = 10 KJ

Burn propagation



Fuel assembly,  
transport, burn-physics



## Several physical models are important for manipulating HED matter to ignition

**Laser Energy = 1.3 MJ**

Opacity, laser-plasma interaction, heat & e-transport

**X-ray Energy = 1 MJ**

Ablator opacity & EOS, drive Spectrum, radiation, e- production & transport

**Energy to capsule = 120 kJ**  
**Set adiabat**

Ablator opacity, drive spectrum, heat & radiation transport, CH & DT EOS

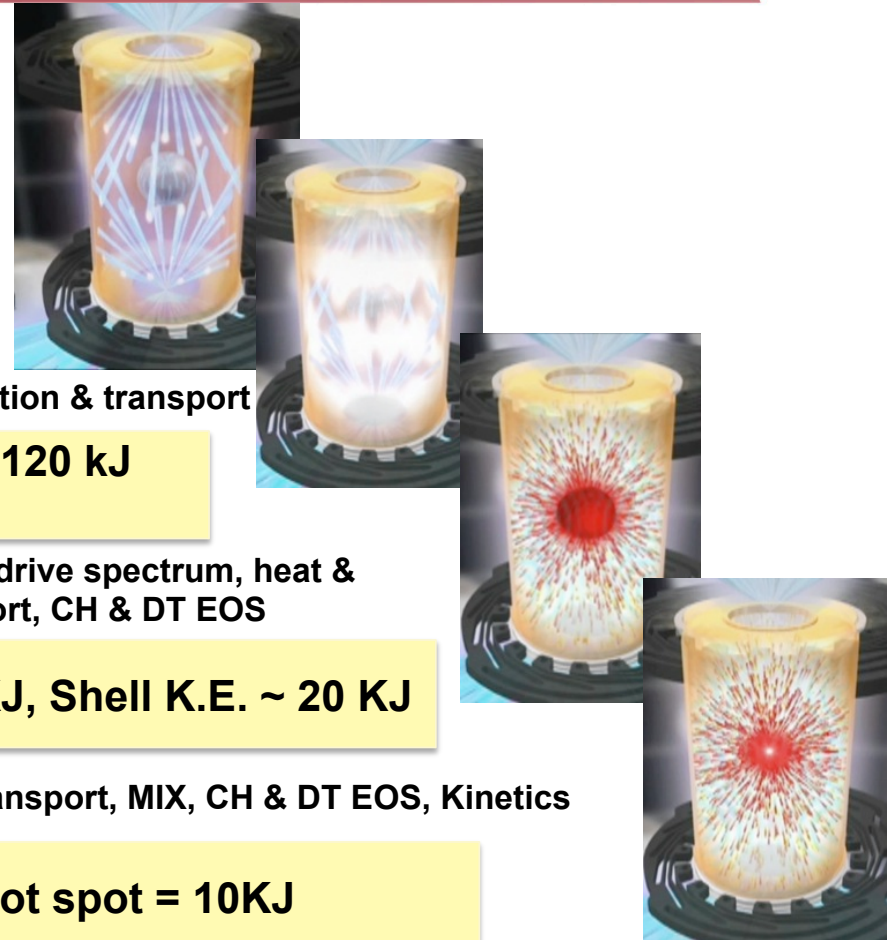
**Fuel K.E. = 12 KJ, Shell K.E. ~ 20 KJ**

Heat transport, MIX, CH & DT EOS, Kinetics

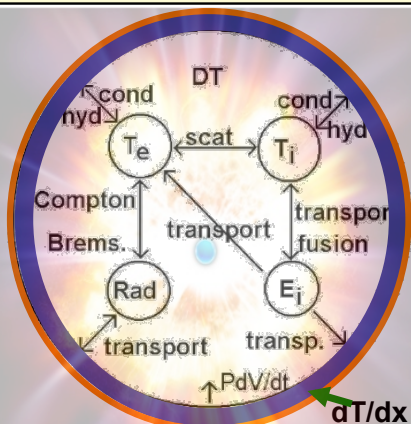
**Hot spot = 10KJ**

Transport, MIX, CH& DT EOS, Bremsstrahlung, reaction rates, Kinetics

**Burn propagation**



**Fuel assembly, transport, burn-physics**





## Several NIC discoveries are motivating improvements in our physical models

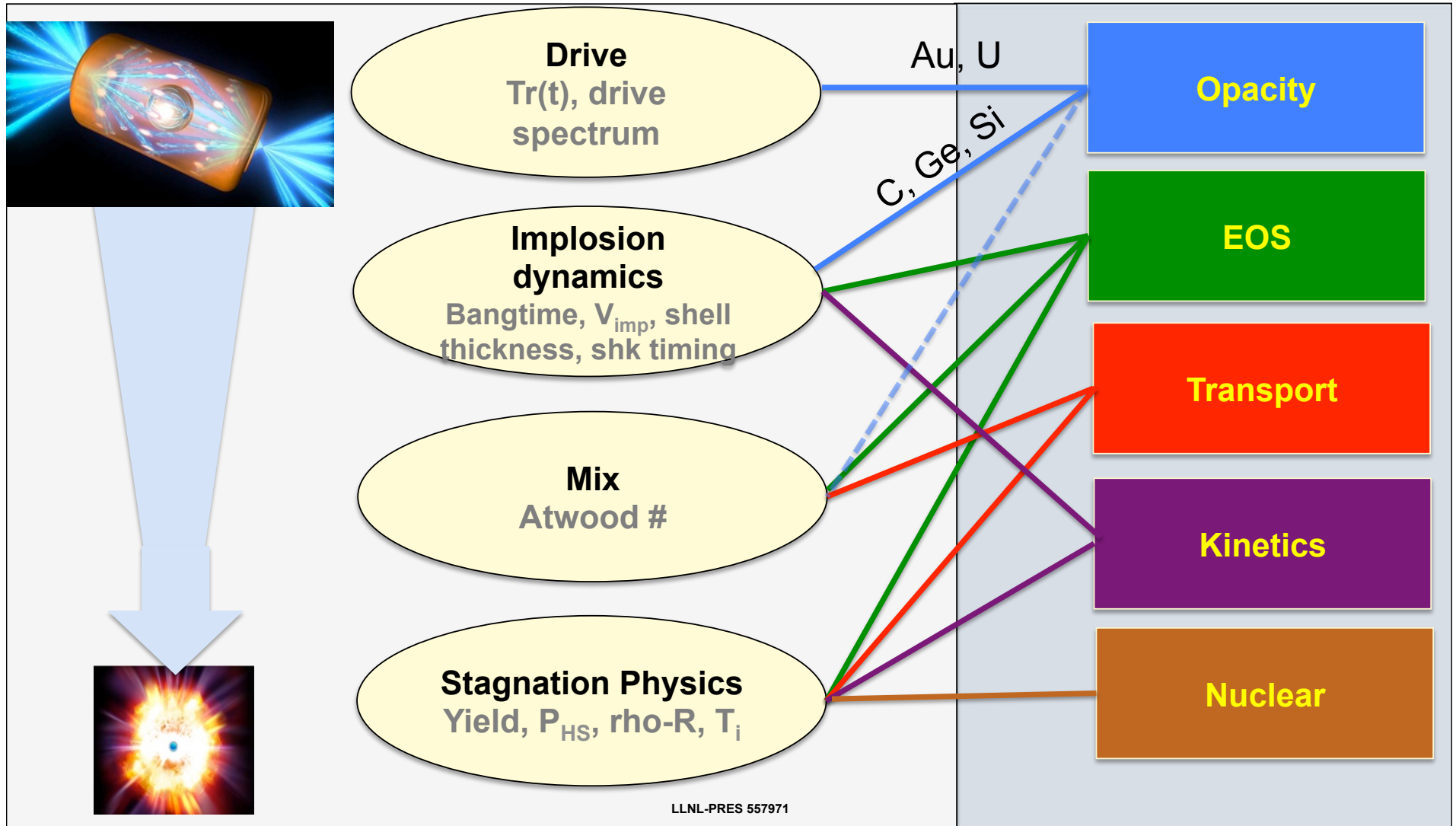
---

- **Drive and ablation physics:**
  - **Implosion velocity,  $V_{\text{imp}}$ , is low** (EOS, Opacity, drive, Kinetics)
  - **$V_{\text{imp}}$  difference between Si and Ge capsules** (Opacity, drive)
  - **Ablator is thicker than predicted** (EOS, NLTE, e- transport)
  - **Ablator release into D2 shows was initially off** (EOS)
  - **Matching shock timing data with simulations requires drive multipliers** (EOS, Opacity, drive, LPI)
- **Stagnation Physics and Mix:**
  - **Yield for a given  $V_{\text{imp}}$  and  $\rho$ -R is low** (EOS, Kinetics, transport)
  - **Hot spot pressure is low** (EOS, Kinetics, transport)
  - **More low energy neutrons (<9MeV) than expected** (Nuclear, kinetics)
  - **$\tau_{\text{Nuclear Burnwidth}} > \tau_{\text{x-ray burnwidth}}$  (transport)**
  - **Mix cliff occurs at higher ablator mass than expected** (Transport, kinetics)

# Our panel will break up into groups focused on physical models, in contrast to implosion stages

## Implosion Performance and NIC Observables

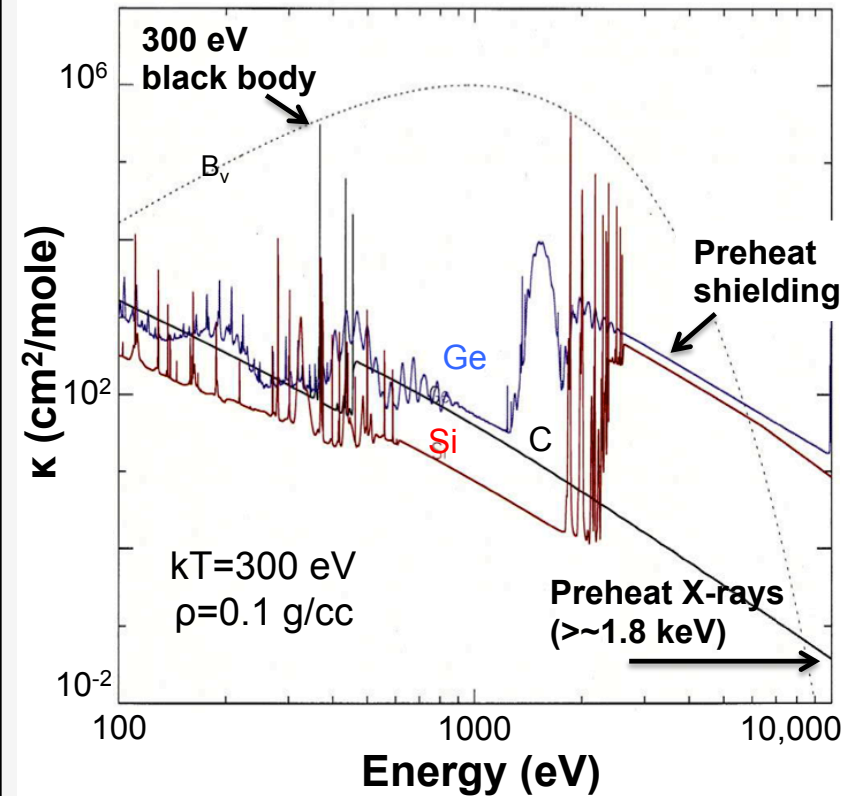
## Physical models



# Optimizing implosion performance requires accurate opacities and emissivities (Si, C, Ge, Au, U)

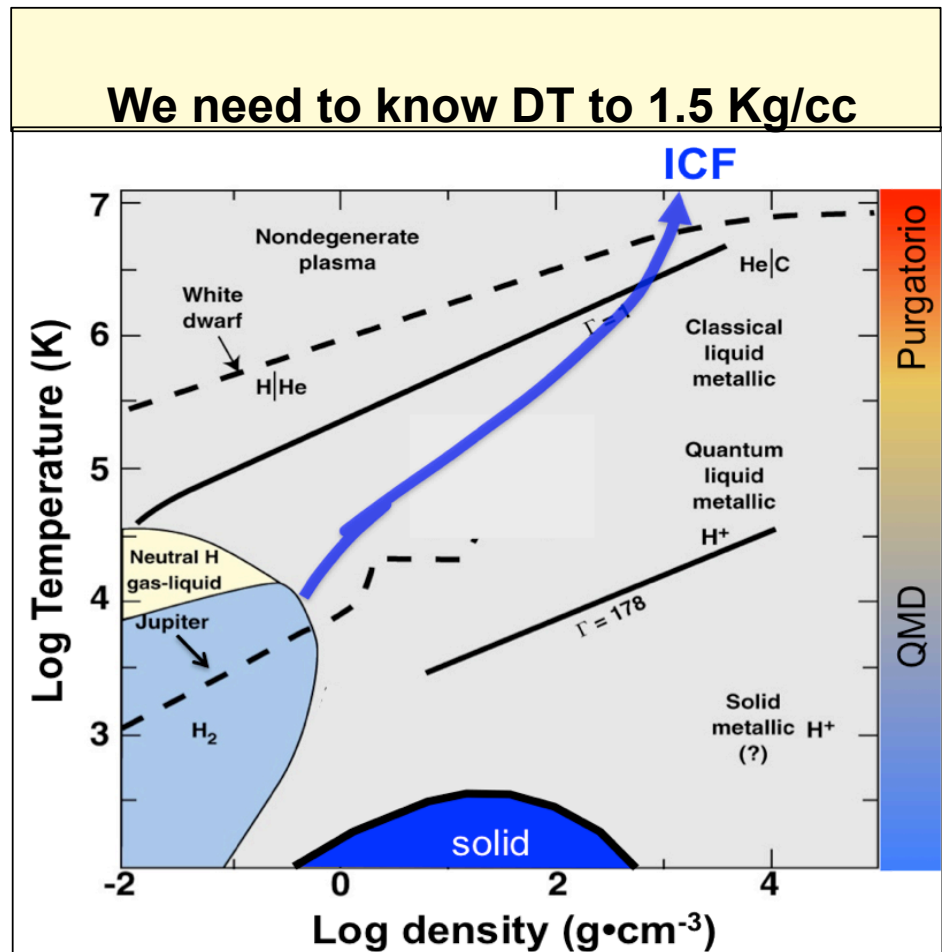
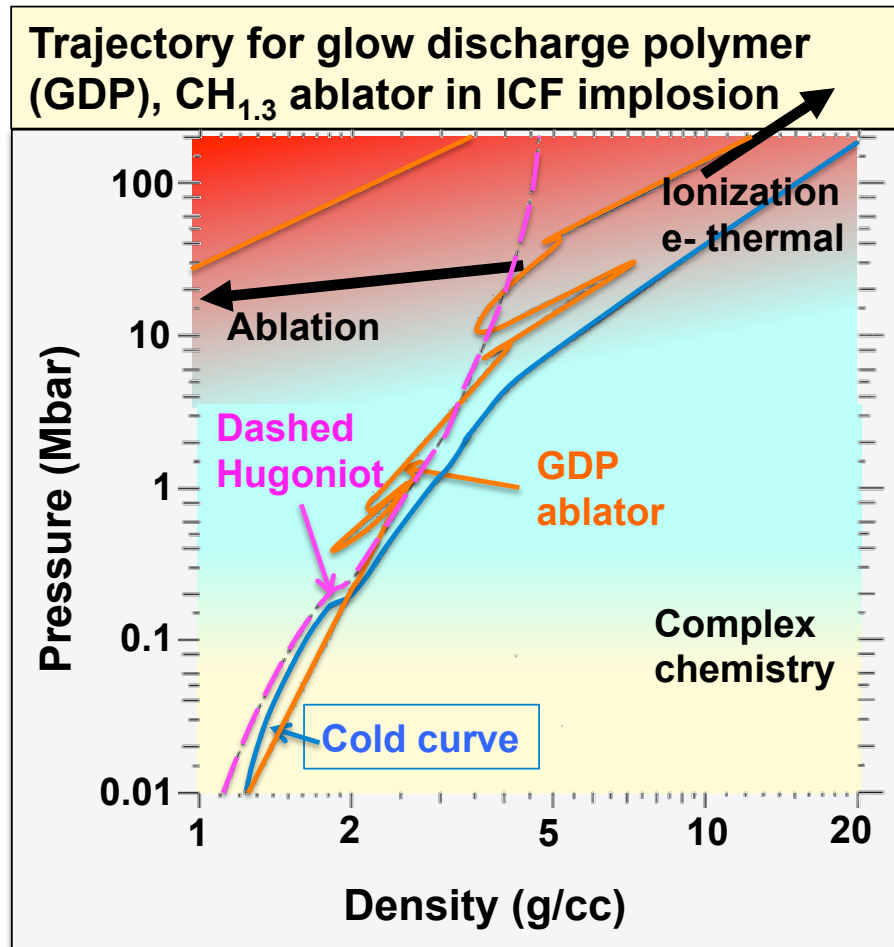
- Ablator opacity (C, Si, Ge) is important for tuning ablation performance, mix and preheat.
- Both NLTE and LTE opacities have been improved recently (H. Scott, S. Hansen, HEDP 6, (2010). B.G. Wilson, et al *PRE* 76, 032103 (2007). ) but still DCA differs from more sophisticated models and EOS and Opacity are not self consistent.
- Important to consider convergence effects in photon binning and material zoning while considering effects of Opacity (Hill and Rose).

C, Ge and Si opacity at .1g/cc and 300 eV





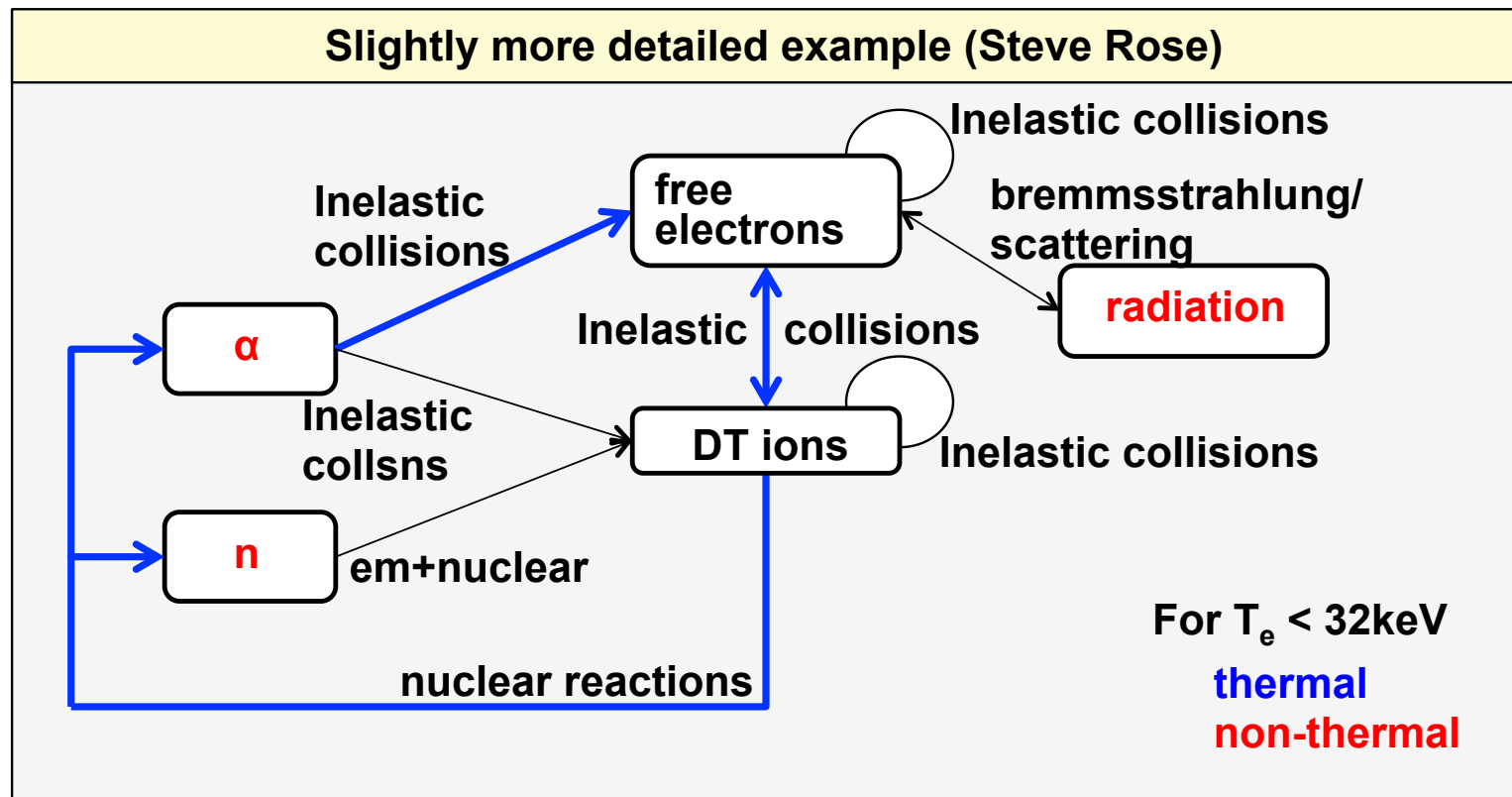
# ICF requires knowledge of the hohlraum, ablator and fuel EOS over a broad range of conditions



Other ablator candidates include diamond, Be,  $\text{B}_4\text{C}$ , Al

## Transport processes implicit to forming a burning plasma are largely untested in relevant regimes

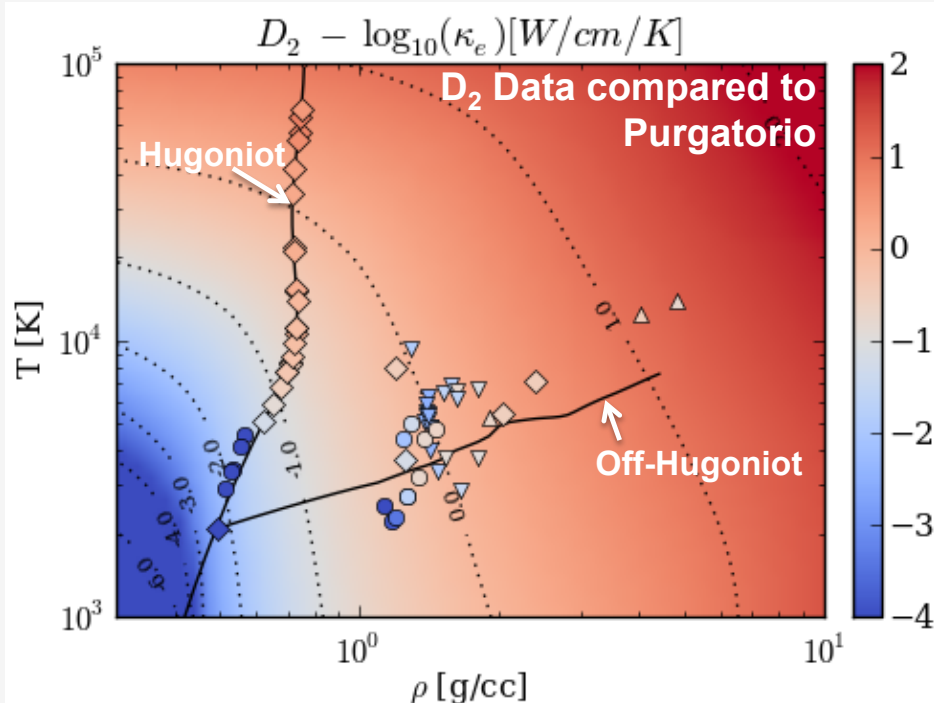
- e-ion coupling in hot spot & dense fuel:
- Stopping power in hot spot & dense fuel:
- Thermal conductivities hot spot & dense fuel:
- Thermal conductivities in CH
- Viscosity models.....
- How to handle mixtures.....
- Bremsstrahlung
- Compton scattering





# Thermal conductivity is important for predicting mix and hotspot dynamics

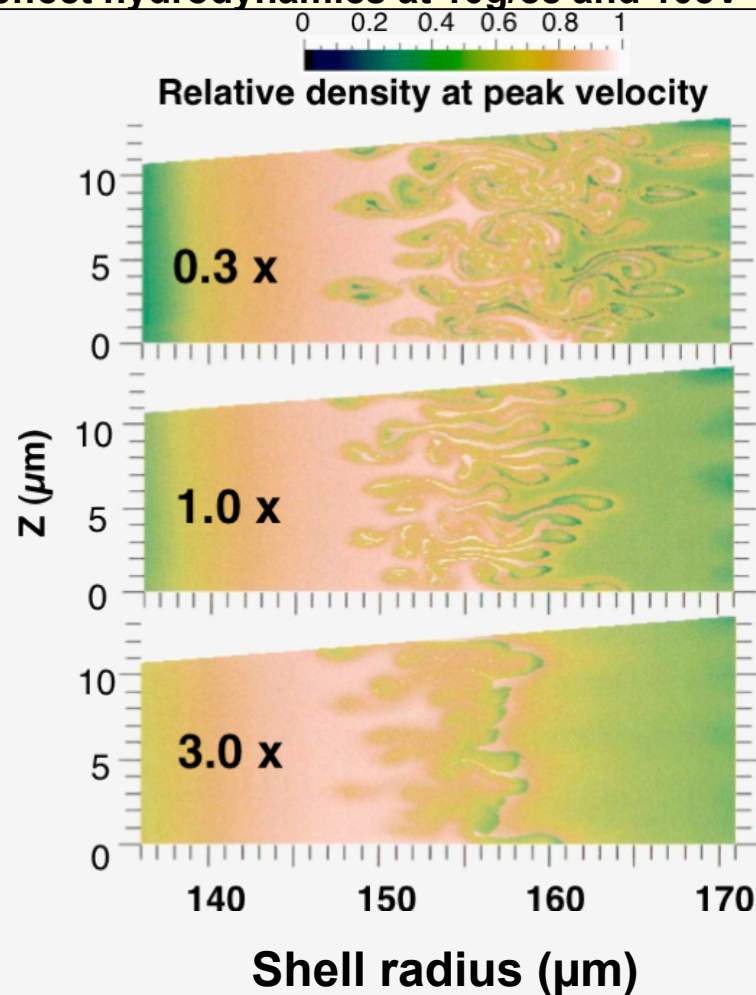
Purgatorio and QMD are in good agreement with D2 data on-Hugoniot but not off-Hugoniot



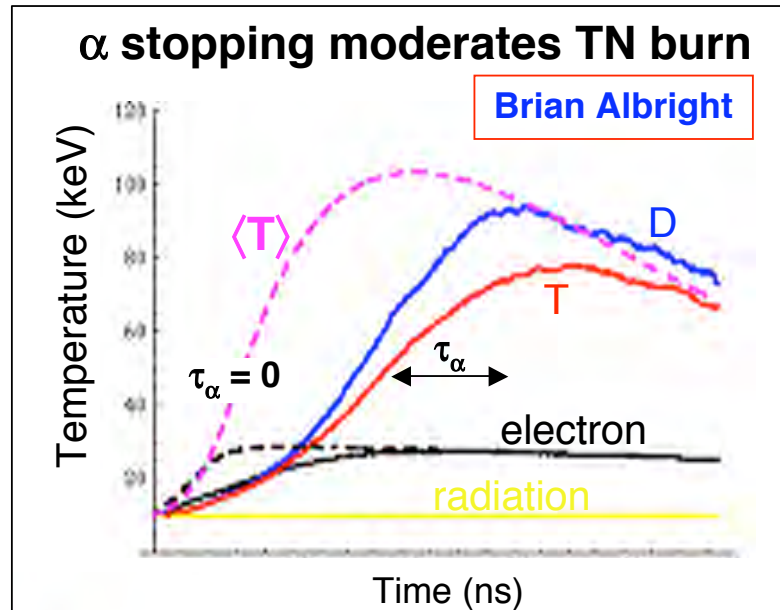
Experimental data:  
 Nellis1992, ○ Nellis1999, ○  
 Celliers2000, ◇ Fortov2003, △  
 Ternovoi2009, ▽ This work ◇

Theory:  
 Purgatorio from  
 Sterne et al.

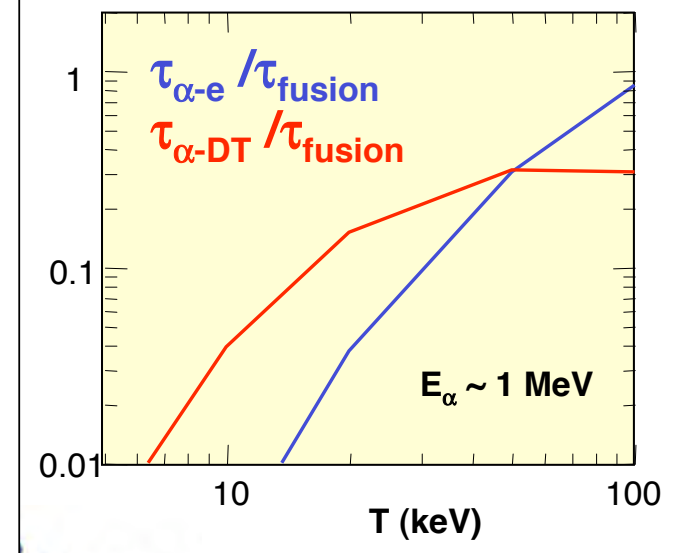
Variations in thermal conductivity of a few times effect hydrodynamics at 10g/cc and 10eV



## Thermonuclear burn in DT involves many complex processes of comparable time scales that compete with confinement time



**$\alpha$ 's couple first to electrons, then to ions as T increases**



**G. Dimonte et al**

**Use VPIC code to simulate infinite  
D-T plasma @  $\rho = 100 \text{ g/cc}$ ,  $T = 10 \text{ keV}$**

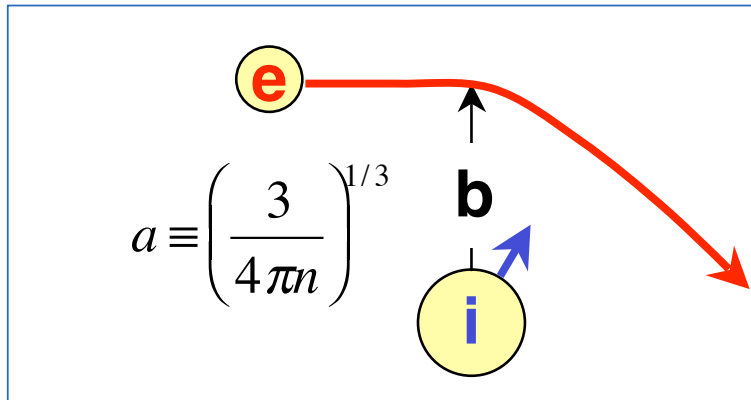
Bowers et al., Phys Plasma **15**, 55703 (08)

Kinetic ions, D, T,  $\alpha$ 's

Fluid electrons

Radiation energy sink

# Electron ion equilibration is important for hotspot dynamics, shock equilibration, and laser coupling



Particle collisions can be described by integrating Rutherford cross-section in Boltzman equation, but this diverges due to distant encounters

Plasma fluctuations due to discrete electrons & ions are described by Lenard-Balescu, but this diverges due to close encounters

$$\frac{dT_i}{dt} \sim \nu_{ie} (T_e - T_i)$$

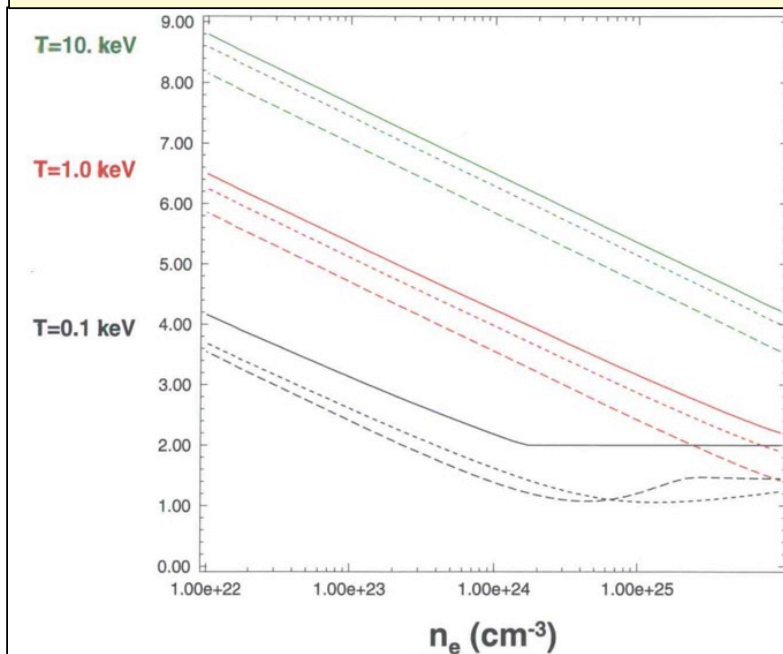
$$\nu_{process} \sim \nu_o \ln \Lambda_{process} \propto \frac{n}{T_e^{3/2}} \ln \left( \frac{b_{\max}}{b_{\min}} \right) \text{ (relativistic correction)(degeneracy correction)}$$

$$\Lambda_{ei}^2 = \frac{\lambda_D^2 + r_i^2}{b_{90}^2 + (\lambda_{dB}/2)^2}$$

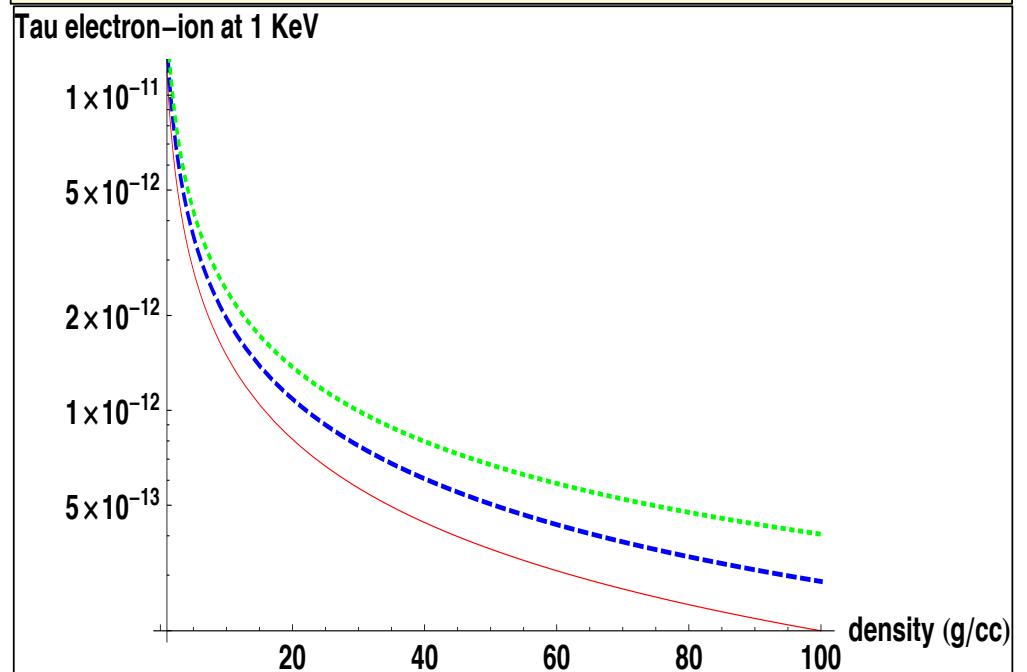
- Lee & More, Phys Fluids, 27, 1273 (1984) includes simple models for degeneracy & limits on impact parameters

# Electron ion equilibration is important for hotspot dynamics, shock equilibration, and laser coupling

Log( $\Lambda$ ) for hydrogen Lee and More (solid), GMS (dotted), BPS(dashed)



Electron ion equilibration time for Lee and More (red), GMS(blue), and BPS (green)



Equilibration times are ~ps while burn durations 10-100 ps

# Stopping of charged particles is dominated by electron-ion interactions and contains ion-ion scattering

Alpha  
stopping

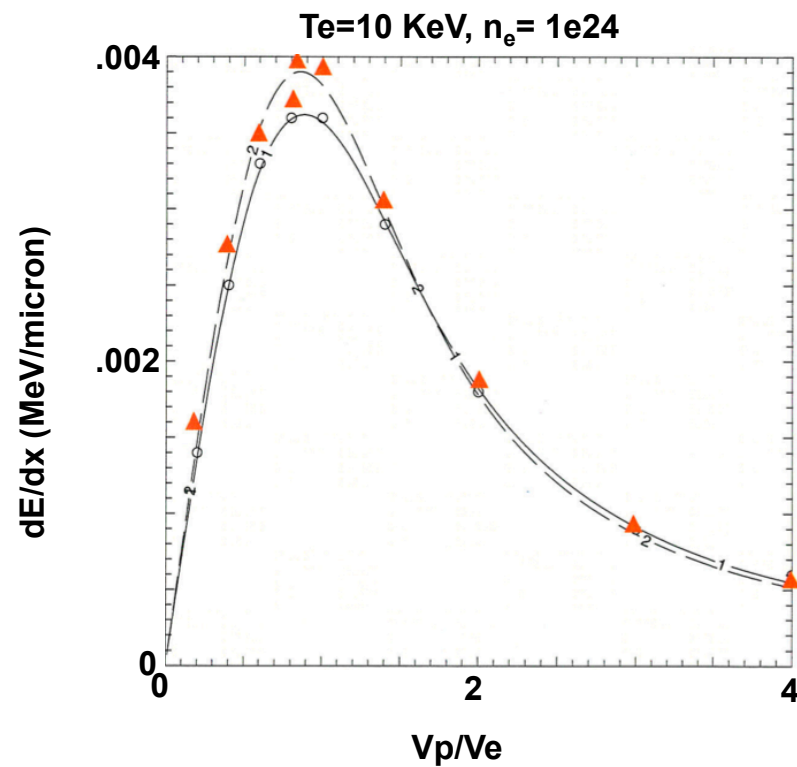
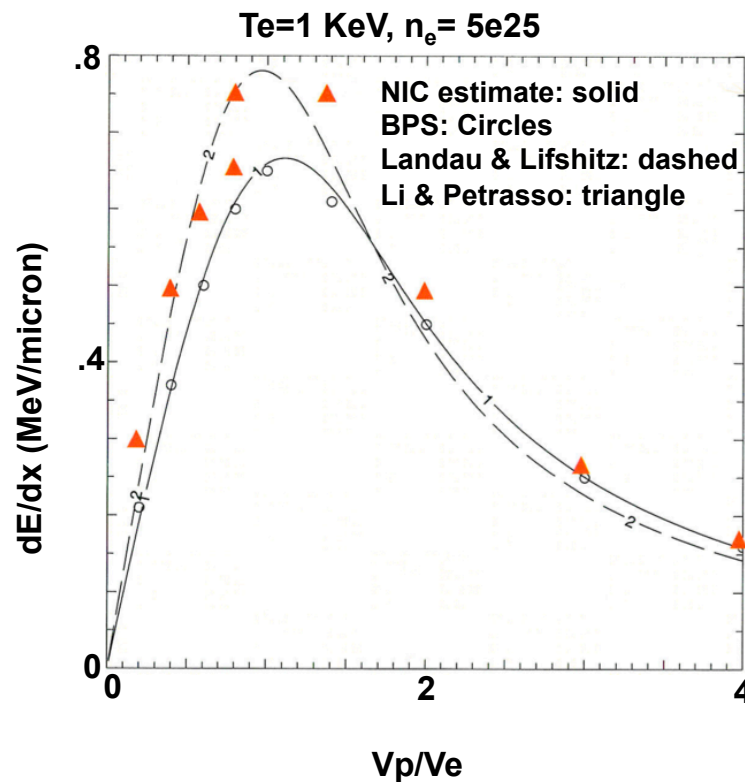
Contribution from  
Ions

Free e-

Bound e-

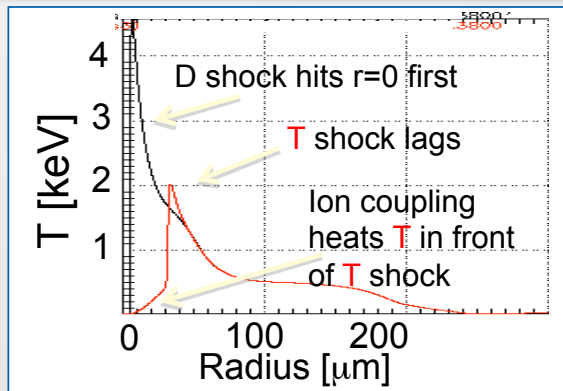
$$\frac{dE}{dx} = C_{ion} \left. \frac{dE}{dx} \right|_i + C_{ion} \left. \frac{dE}{dx} \right|_e + C_{ion} \left. \frac{dE}{dx} \right|_b$$

- Zimmerman, UCRL-JC-105616 (1990)
- Maynard & Deutsch, J. Physique, 46, 1113 (1985)



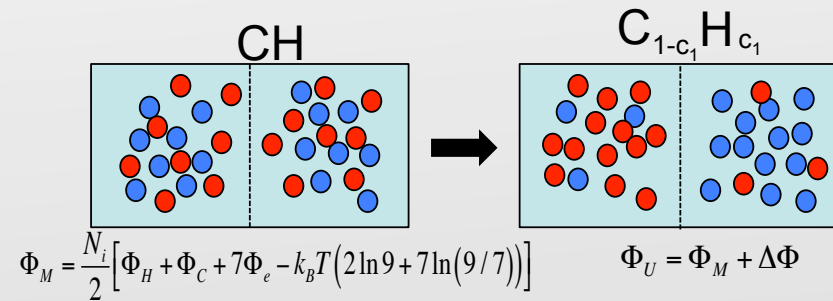
# Summary of candidate multi-species and kinetic effects

## Shock Separation



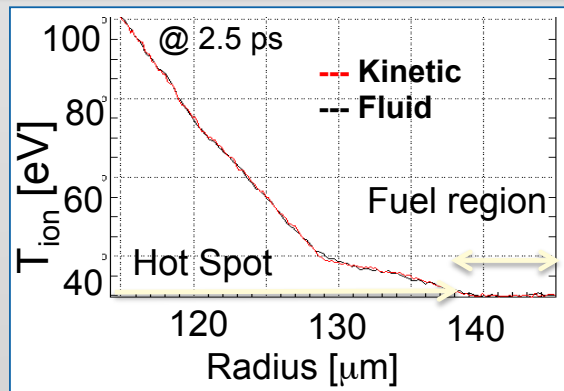
Pressure gradient-induced  $E$ -field causes lighter species to accelerate ahead of heavier species

## Species Separation in Ablator



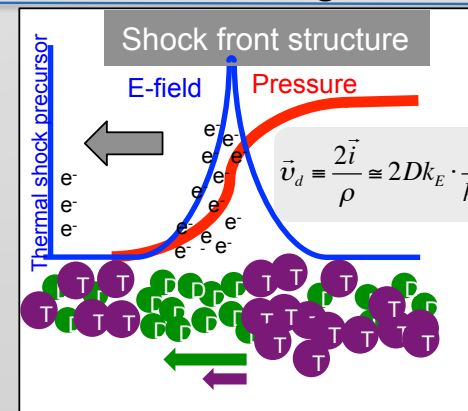
Some fraction of ablation energy goes into separating C from H, resulting in loss of ablation efficiency

## Heating Due to Tail of Distribution



During hot spot formation, electrons in tail of energy distribution ( $\sim 10 \times T_e$ ) may heat fuel

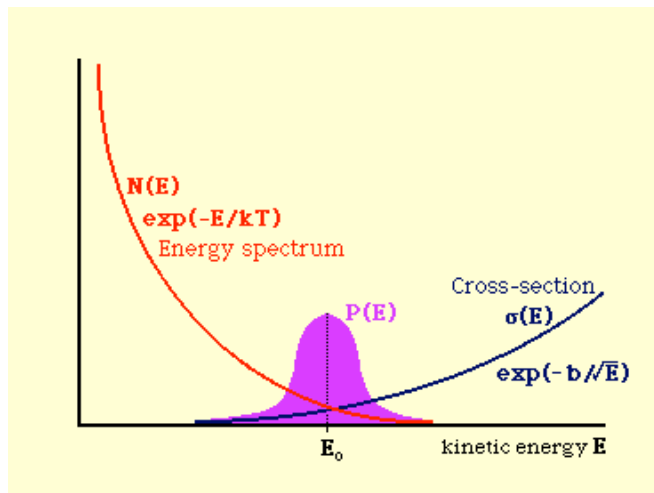
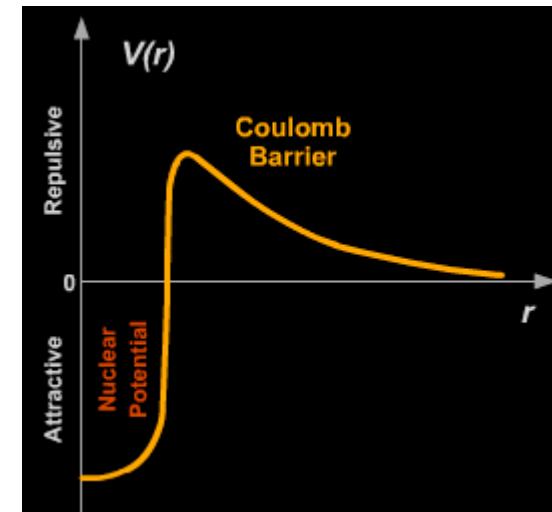
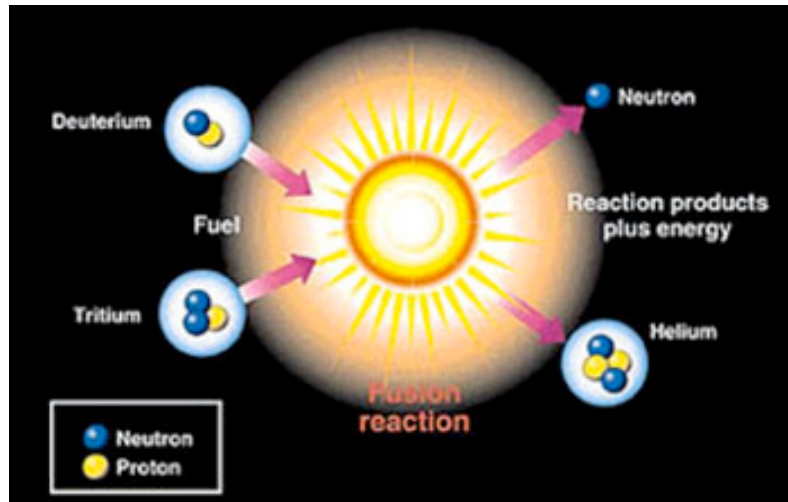
## Frictional Shock Heating of DT



Shocks in dense plasma cause relative drift speed between species: energy in directed  $V$  goes into heat



# Thermonuclear Burn as well as nuclear diagnostic data interpretation depend on nuclear reaction rates



D-T reaction rate is extremely dependent on  $T_{\text{ion}}$ .

$\alpha$ -particles can heat up electrons and ions differently.



# The first nuclear cross section measurement using an ICF facility has been made at Omega

PRL 107, 122502 (2011) PHYSICAL REVIEW LETTERS week ending 16 SEPTEMBER 2011

## Measurements of the Differential Cross Sections for the Elastic $n$ - $^3\text{H}$ and $n$ - $^2\text{H}$ Scattering at 14.1 MeV by Using an Inertial Confinement Fusion Facility

J. A. Frenje, C. K. Li, F. H. Seguin, D. T. Casey, and R. D. Petrasso

*Plasma Science and Fusion Center, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

D. P. McNabb, P. Navrátil, and S. Quaglioni

*Lawrence Livermore National Laboratory, Livermore, California 94550, USA*

T. C. Sangster, V. Yu Glebov, and D. D. Meyerhofer\*

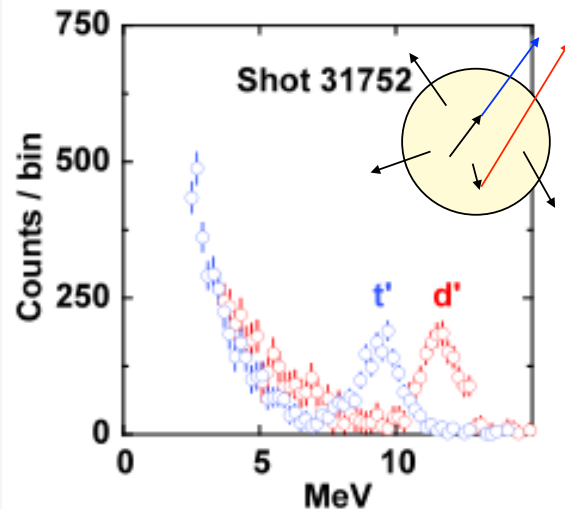
*Laboratory for Laser Energetics, University of Rochester, Rochester, New York 14623, USA*

(Received 18 June 2011; published 15 September 2011)



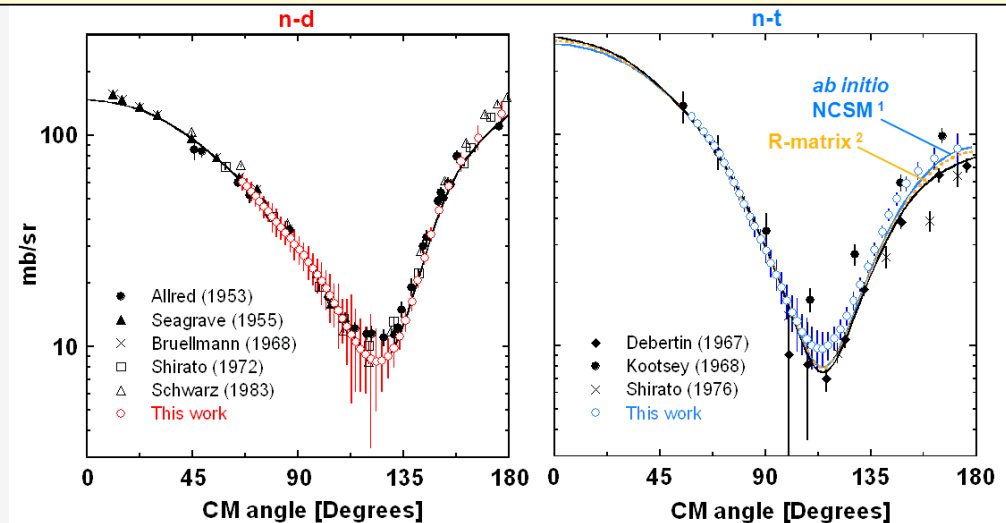
### n-D,T Elastic Scattering

Plasma is neutron source and target



Simultaneous measurements of d' and t' spectra scattered by d-t neutrons.

### Comparison with ab initio calculations

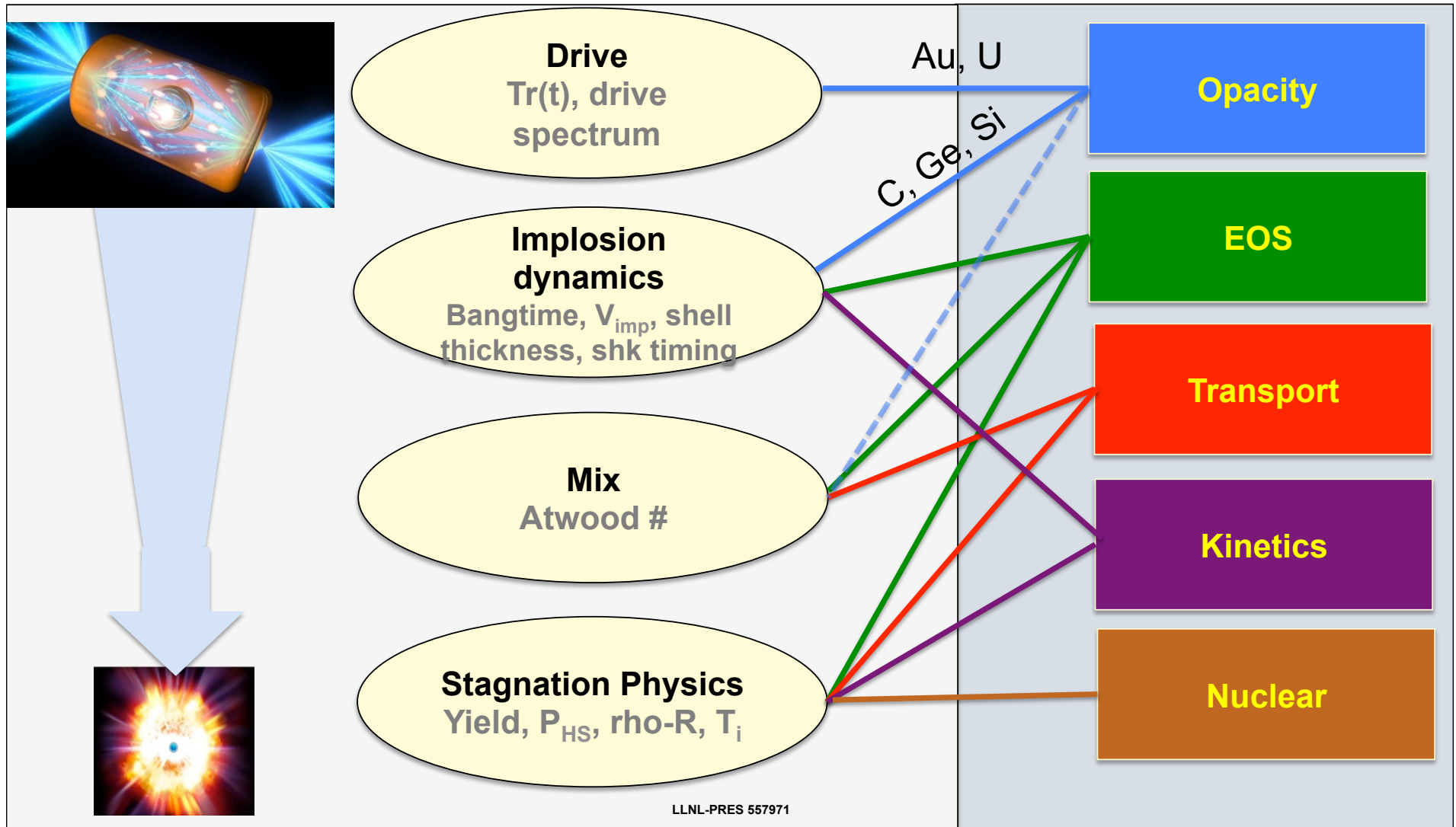


1. P. Navrátil et al., LLNL-TR-423504 (2010).
2. Ga.A. Hale et al., Phys. Rev. C 42, 438 (1990).

# Next several talks will outline each of the physics models in the codes. What are we missing?

## Implosion Performance and NIC Observables

## Physical models



# NIC

**Details of our electron ion equilibration and  
stopping power follow in the next 6 vgs**



## Details for electron ion equilibration model used in NIC calculations

- Includes degeneracy, partial ionization, relativity, Lee & More  $\ln(\Lambda)$

$$\frac{de}{dt} = M_1 \cdot 8\alpha^2 \frac{m_e}{m_p} \frac{m_e c^2}{h} \frac{\text{"ln"}(\Lambda_{ei})}{(1 + e^{-\mu/T_e})} \left( \sum_i n_i \frac{z_i^{*2}}{A_i} \right) k(T_i - T_e) R(M_2 \frac{kT_e}{m_e c^2})$$

$$R(\tau) = \frac{K_{1/2}(1/\tau) + 2\tau K_{3/2}(1/\tau)}{K_2(1/\tau)}$$

$$\text{"ln"}(\Lambda) = \max \left[ \logmin, \frac{1}{2} \ln(1 + M_3 \Lambda^2) - C_1 + C_2 / \Lambda \right]$$

$$M_3 = M_3(\text{reg}) \frac{z^* + C_{3N}}{z^* + C_{3D}}$$

Many knobs to test sensitivities

## Log $\Lambda_{ei}$ is largely from Lee and More

- Lee & More, Phys Fluids, 27, 1273 (1984) includes simple models for degeneracy & limits on impact parameters

What is  $r_i$  for a mixture?

$$\Lambda_{ei}^2 = \frac{\lambda_D^2 + r_i^2}{b_{90}^2 + (\lambda_{dB}/2)^2}$$

When should ions be included?

$$\frac{4}{3}\pi r_i^3 = \frac{1}{n_i}$$

$$\frac{1}{\lambda_D^2} = 4\pi e^2 \left( \frac{n_e}{kT_b} + \frac{\sum n_i z_i^{*2}}{kT_i} \right)$$

$$b_{90} = z^* e^2 / m_e v_b^2$$

$$\lambda_{dB} = \hbar / m_e v_e$$

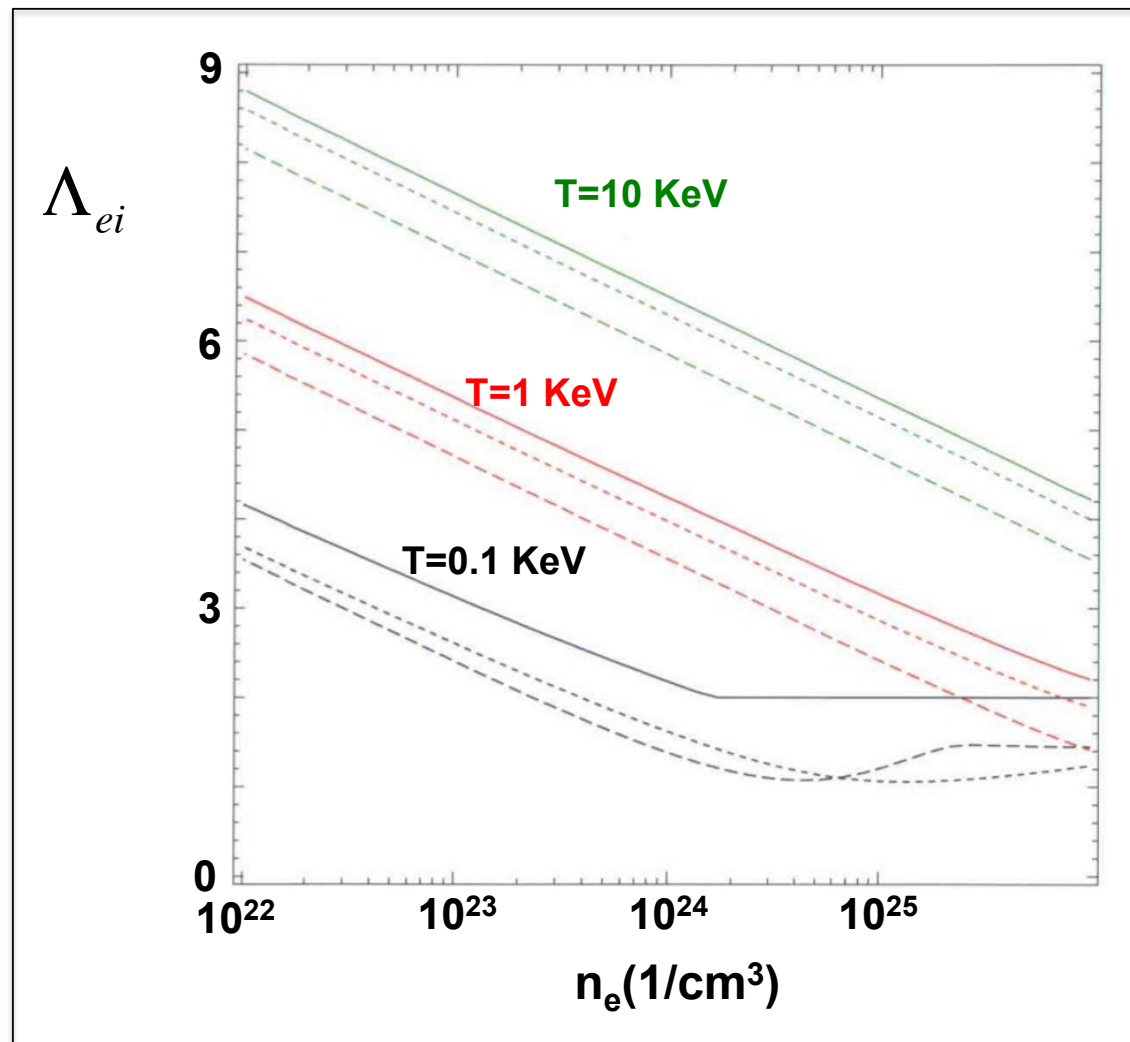
$$\frac{1}{2} m_e v_b^2 = \frac{3}{2} kT_b$$

$$T_b^2 = T_e^2 + (2/3 E_F)^2$$

$$z^* = \sum n_i z_i^{*2} / n_e$$



# Log( $\Lambda_{ei}$ ) for hydrogen: Lee & More (solid), GMS6 (dotted), BPS (dashed)



# Stopping of charged particles is dominated by electron-ion interactions and contains ion-ion scattering

Alpha  
stopping

Contribution from  
Ions

Free e-

Bound e-

$$\frac{dE}{dx} = C_{ion} \left. \frac{dE}{dx} \right|_i + C_{ion} \left. \frac{dE}{dx} \right|_e + C_{ion} \left. \frac{dE}{dx} \right|_b$$

Ion contribution is small except at very high Te or electron density

$$\left. \frac{dE}{dx} \right|_i = \frac{4\pi e^2 z_p^2}{v_p^2} \sum \frac{n_i z_i^2}{m_i} \ln(\lambda_D / b_i)$$

$$\lambda_D^2 = \frac{kT_e}{4\pi e^2 n_e}$$

$$b_i^2 = \left( \frac{\hbar}{2m_r v_p} \right)^2 + \left( \frac{e^2 z_i z_p}{m_r v_p^2} \right)^2$$

Ions not included

- Zimmerman, UCRL-JC-105616 (1990)
- Maynard & Deutsch, J. Physique, 46, 1113 (1985)

# Stopping of charged particles is dominated by electron-ion interactions and contains ion-ion scattering

Alpha  
stopping

Contribution from  
Ions

Free e-

Bound e-

$$\frac{dE}{dx} = C_{ion} \left. \frac{dE}{dx} \right|_i + C_{ion} \left. \frac{dE}{dx} \right|_e + C_{ion} \left. \frac{dE}{dx} \right|_b$$

Free electron stopping includes degeneracy and full range of ion-e- velocities

Bound electron stopping uses average excitation energy from More UCRL-84991, Sec VII

$$\left. \frac{dE}{dx} \right|_e = \frac{4\pi e^2 z_p^2}{m_e v_p^2} n_e L_e$$

$$L_e = \frac{1}{2} \ln(\Lambda_e) \left( \operatorname{erf}(y) - \frac{2}{\sqrt{\pi}} y e^{-y^2} \right)$$

$$\Lambda_e = \frac{2m_e v_e^2}{\hbar \omega_{pe}} \cdot \frac{0.321 + 0.259y^2 + 0.0707y^4 + 0.05y^6}{1 + 0.130y^2 + 0.05y^4}$$

$$y = v_p / v_e$$

$$v_e = \sqrt{\pi} \frac{\hbar}{m_e} \left( 4n_e \left( 1 + e^{-\mu/T_e} \right) \right)^{1/3}$$

$$\left. \frac{dE}{dx} \right|_b = \frac{4\pi e^2 z_p^2}{m_e v_p^2} \sum n_i z_{ib} L_{ib}$$

$$z_{ib} = z_i - z_i^*$$

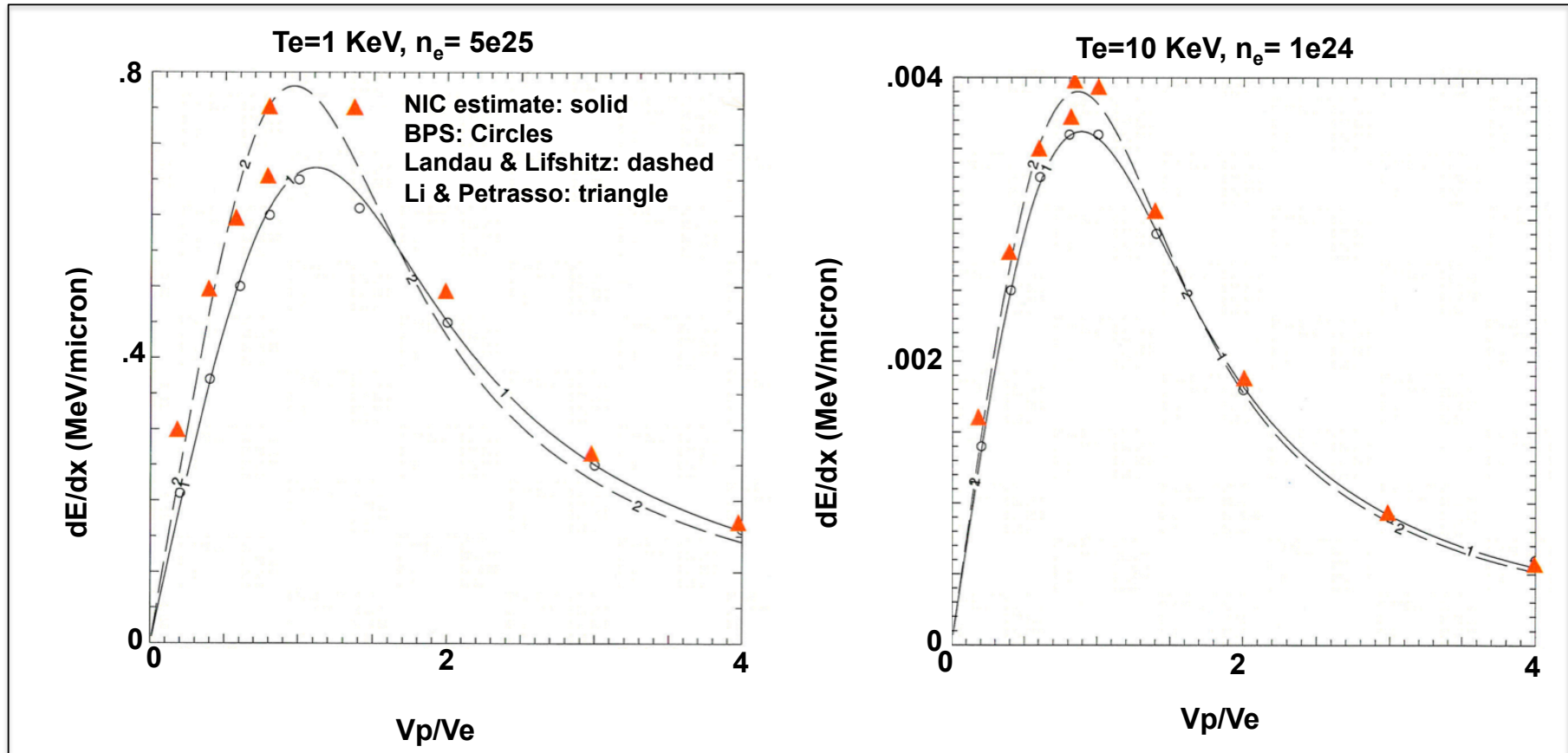
$$L_{ib} = \frac{1}{2} \ln(1 + \Lambda_b^2)$$

$$\Lambda_b = 2m_e v_p^2 / \bar{I}_i$$

$$\bar{I}_i = z_i \frac{0.024 - 0.013(z_{ib} / z_i)}{\sqrt{z_{ib} / z_i}} \quad \text{keV}$$



## For burn conditions $dE/dx$ used in ignition calculations agree with Brown, Preston and Singleton





# NIC

**End of Intro talk**

